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A framework to evaluate and elucidate the driving mechanisms of coastal sea surface pCO₂ seasonality using an ocean general circulation model (MOM6-COBALT)

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Abstract

The temporal variability of the sea surface partial pressure of CO_2 (pCO_2) and the underlying processes driving this variability are poorly understood in the coastal ocean. In this study, we tailor an existing method that quantifies the effects of thermal

15 changes, biological activity, ocean circulation and fresh water fluxes to examine seasonal pCO_2 changes in highly-variable coastal environments. We first use the Modular Ocean Model version 6 (MOM6) and biogeochemical module Carbon Ocean Biogeochemistry And Lower Trophics version 2 (COBALTv2) at a half degree resolution to simulate the coastal CO_2 dynamics and evaluate it against pCO_2 from the Surface Ocean CO_2 Atlas database (SOCAT) and from the continuous coastal pCO_2 product generated from SOCAT by a two-step neuronal network interpolation method (coastal-SOM-FFN, Laruelle et al.,

20 2017). The MOM6-COBALT model not only reproduces the observed spatio-temporal variability in pCO_2 but also in sea surface temperature, salinity, nutrients, in most coastal environments except in a few specific regions such as marginal seas. Based on this evaluation, we identify coastal regions of 'high' and 'medium' model skill where the drivers of coastal pCO_2 seasonal changes can be examined with reasonable confidence. Second, we apply our decomposition method in three contrasted coastal regions: an Eastern (East coast of the U.S) and a Western (the Californian Current) boundary current and a

25 polar coastal region (the Norwegian Basin). Results show that differences in pCO_2 seasonality in the three regions are controlled by the balance between ocean circulation, biological and thermal changes. Circulation controls the pCO_2 seasonality in the Californian Current, biological activity controls pCO_2 in the Norwegian Basin, while the interplay between biology, thermal and circulation changes is key in the East coast of the U.S. The refined approach presented here allows the attribution of pCO_2 changes with small residual biases in the coastal ocean, allowing future work on the mechanisms controlling coastal

30 air-sea CO_2 exchanges and how they are likely to be affected by future changes in sea surface temperature, hydrodynamics and biological dynamics.

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1 Introduction

The ocean plays an important role in offsetting human-induced carbon dioxide (CO_2) emissions associated with cement production and fossil fuel combustion (Friedlingstein et al., 2019). Globally, the ocean is a net sink that absorbs roughly one

35   quarter of the anthropogenic CO_2 emitted into the atmosphere (-2.5 ± 0.6 Petagram of carbon per year (Pg C yr^{-1}) for the 2009-2018 decade, Friedlingstein et al., 2019). The spatio-temporal variability of this oceanic CO_2 uptake is relatively well constrained in the open ocean thanks to several method including sea surface CO_2 data-derived interpolations (e.g., Landschützer et al., 2014; Rödenbeck et al., 2014, 2015; Takahashi et al., 2002), models and atmospheric inversions (e.g., Gruber et al., 2009, 2019; Keeling and Manning, 2014; Manning and Keeling, 2006), but it is less constrained and understood

40   in the coastal ocean. Nonetheless, in recent decades, significant progress have been made with regard to the quantification and analysis of the spatial distribution of the coastal air-sea CO_2 exchange (FCO$_2$) globally and regionally (e.g., Borges et al., 2005; Cai, 2011; Chen et al., 2013; Laruelle et al., 2010, 2014, Roobaert et al., 2019). The FCO$_2$ seasonal cycle was also recently analyzed in coastal regions worldwide by Roobaert et al. (2019). This study identified that at the annual timescale, the global coastal ocean acts as an atmospheric CO_2 sink (-0.2 ± 0.02 Pg C yr^{-1}) with a more intense CO_2 uptake occurring in summer

45   because of the disproportionate influence of high latitude coastal seas in the Northern Hemisphere. A more in-depth analysis also revealed that the majority of the coastal seasonal FCO$_2$ variations stems from the air-sea gradient in partial pressure of CO_2 (pCO$_2$), although changes in wind speed and sea-ice cover can be significant regionally.

Several processes influence the seasonal variations of surface ocean pCO$_2$ and thus, the seasonality in FCO$_2$. These processes

50   include changes in sea surface temperature (SST) tied to air-sea heat fluxes and ocean circulation, changes in sea surface salinity (SSS) associated with evaporation, fresh water fluxes (from land, ice-melt, precipitation and evaporation) and ocean circulation, as well as variations in sea surface alkalinity (ALK) and dissolved inorganic carbon (DIC) tied to biological activity, fresh water fluxes and ocean circulation (Sarmiento and Gruber, 2006). In the open ocean, the respective influence of these processes on the pCO$_2$ variability has been interpreted using changes in SST, SSS, ALK and DIC observed in-situ (e.g.,

55   Landschützer et al., 2018; Takahashi et al., 1993) or based on global/regional ocean biogeochemical models relying on a mechanistic, quantitative description of the physical, chemical and biological processes controlling the ocean carbon cycle (e.g., Doney et al., 2009). These investigations reveal that changes in SST (i.e. the thermal effect) is the main driver of the seasonal pCO$_2$ in tropical oceanic regions, while non-thermal components (change associated with DIC, ALK and SSS) dominate at mid- and high-latitude (poleward of 40° N and 40° S, e.g., Landschützer et al., 2018; Takahashi et al., 2002).

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In the coastal ocean, the processes controlling the pCO$_2$ seasonal dynamics was mostly investigated regionally (e.g., Arruda et al., 2015; Frankignoulle & Borges, 2001; Laruelle et al., 2014; Nakaoka et al., 2006; Shadwick et al., 2010, 2011; Signorini et al., 2013; Turi et al., 2014; Yasunaka et al., 2016) and only a few observation-based studies attempted to analyze the coastal pCO$_2$ seasonal variability into processes at the global scale (Cao et al., 2020; Chen and Hu, 2019; Laruelle et al., 2017).

65   Regional studies using either observations or model results have covered, e.g., the shelves of the entire Atlantic basin (Laruelle et al., 2014), the West (California Current, Turi et al., 2014) and East (e.g., Shadwick et al., 2010, 2011; Signorini et al., 2013) coasts of the United States, as well as the South and Southeast Brazilian shelves, Uruguayan and Patagonia shelves and shelves along the southwestern Atlantic ocean (Arruda et al., 2015). In the California Current, the strong upwelling of carbon-rich waters was identified as the main control of the pCO_2 seasonality (Turi et al. 2014). On the Patagonia shelf, the thermal effect

70   and biological pumps were found to be the main drivers of the seasonal pCO_2 variability with only a small contribution from the ocean circulation (Arruda et al., 2015), while along the East coast of the U.S, seasonal thermal changes play the major role (Shadwick et al., 2010, 2011; Laruelle et al., 2015; Signorini et al., 2013). These studies are, however, confined to specific regions and a global picture of the mechanisms driving the coastal pCO_2 dynamics is still missing. In addition, the attribution analysis into specific physical and biological processes is incomplete. Indeed, the attribution relies on a linear decomposition

75   linking variations in sea surface ocean pCO_2 to seasonal changes in DIC, ALK, SST and SSS (e.g., Signorini et al., 2013, Doney et al., 2009; Lovenduski et al., 2007; Takahashi et al., 1993; Turi et al., 2014), or on a series of sequential simulations isolating biological and physical terms therefore ignoring how covariations between the different terms dampen or reinforce each other (e.g., Arruda et al., 2015; Turi et al., 2014).

80   In this study, we develop a new framework to elucidate the seasonal pCO_2 dynamics of the global coastal ocean. This framework relies on the global Modular Ocean Model version 6 (MOM6, Adcroft et al., 2019) from the NOAA Geophysical Fluid Dynamics Laboratory coupled to the biogeochemical module Carbon Ocean Biogeochemistry And Lower Trophics version 2 (COBALTv2, Stock et al., 2014, 2020). MOM6-COBALT model outputs provide the relevant variables and processes that are required to perform an explicit decomposition of the inorganic carbon dynamics (Liao et al., 2020) in the

85   entire coastal domain. These outputs are then analyzed using a novel approach to attribute seasonal variations in surface ocean pCO_2 to changes in biological activity, ocean circulation, SST, air-sea CO_2 fluxes and fresh water fluxes (Liao et al., 2020), and which is here enhanced for the coastal ocean. The decomposition method constitutes a significant improvement upon previous studies. First, it accounts for co-variations in biological and physical processes and how their evolution jointly modulates the pCO_2 signal. Second, it improves on the traditional linear approaches developed for the open ocean (Sarmiento

90   and Gruber, 2006; Takahashi et al., 1993) and used since then (e.g. Lovenduski et al., 2007), because, as shown later in this study, the linear decomposition introducing significant biases in coastal waters due to the larger range in DIC, ALK, pH and salinity values encountered in the variable coastal environment (Egleston et al., 2010).

In light of these knowledge gaps, the objective of this paper are twofold:

95   -   First, we evaluate the performance of the MOM6-COBALT model in its ability to reproduce the observed spatio-temporal fields of SSS, SST, sea surface nutrients and pCO_2 in the global coastal domain. In particular, we identify the coastal regions where the model best reproduces the observed ocean pCO_2 variability and can thus be considered most suitable for a detailed analysis of the drivers of the pCO_2 seasonal changes.

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- Second, to illustrate the capabilities of our upgraded decomposition framework, we examine the drivers of the pCO_2
100   seasonality in three contrasted coastal regions: The East coast of the U.S, the West coast of North America and the
Norwegian Basin.

2 Methodology

2.1 Ocean biogeochemical model description

In this study, we used the ocean model MOM6 and the Sea Ice Simulator version 2 (fourth generation of ocean-ice models
105   called OM4) detailed in Adcroft et al. (2019). The version of OM4 adopted here is OM4p5 which has a nominal horizontal
resolution of 0.5° (i.e. with a finer latitudinal resolution of 0.26° in the tropical region). On the vertical, it includes 75 hybrid
coordinates with a z* coordinate near the surface (geopotential coordinate allowing free surface undulations) and a modified
potential density coordinate below. The vertical spacing increases from 2 m in the upper 20 m (i.e first 10 layers) to larger
isopycnal layers below. Layers in z* broadly deepens towards high latitudes (see Adcroft et al., 2019 for details on the grid).
110   This ocean-ice model is coupled to the biogeochemical module COBALT version 2 (COBALTv2), which includes 33 state
variables to resolve global-scale cycles of carbon, nitrogen, phosphate, silicate, iron, calcium carbonate, oxygen and lithogenic
materials (Stock et al., 2020). Details about the planktonic food web dynamics in COBALT, and global assessments of large-
scale carbon fluxes through the food web such as net primary production can be found in Stock et al. (2014, 2020). The ocean
model is forced by the 55-km horizontal resolution Japanese atmospheric reanalysis (JRA55-do) version 1.3 at a 3-hour
115   frequency between 1959 and 2018 (Tsujino et al., 2018), and the atmospheric pCO_2 data from the Earth System Research
Laboratory (Joos and Spahni, 2008). SST, SSS, sea surface nutrients (nitrate, phosphate, silicate) and oxygen were initialized
from the World Ocean Atlas version 2013 (Garcia et al., 2013a, 2013b; Locarnini et al., 2013; Zweng et al., 2013). Initial DIC
and ALK conditions are taken from GLODAPv2 (Olsen et al., 2016). The initial DIC is corrected for the accumulation of
anthropogenic carbon to match the level expected in the first year of simulation (1959) using the data-based estimate of ocean
120   anthropogenic carbon content of Khatiwala et al. (2013). At the end of a 81-year spin-up repeating year 1959, the model has
reached a near-equilibrium between atmospheric pCO_2 and surface ocean pCO_2, with a drift in global air-sea CO_2 flux < 0.004
Pg C yr^{-1} over the last 10 years of spin-up. Further details on the configuration, spin-up and simulation can be found in Liao et
al. (2020).

2.2 Observational products and model evaluation

125   We first evaluate the ability of MOM6-COBALT to reproduce the observed spatial distribution of environmental variables in
the coastal domain, namely the SST, SSS and sea surface nutrients (nitrate, phosphate and silicate). The observational SST
and SSS fields are from the daily NOAA OI SST V2 (Reynolds et al., 2007) and the daily Hadley center EN4 SSS (Good et
al., 2013), respectively. The observed nutrient fields in the sea surface are extracted from the World Ocean Atlas version 2018
(Garcia et al., 2019). We also compare the simulated coastal pCO_2 directly to "raw", un-interpolated observations extracted

130   from the Surface Ocean CO_2 Atlas database (SOCAT), using monthly observations from SOCAT version 6 gridded at the

spatial resolution of 0.25 degree (SOCATv6, Bakker et al., 2016). For the evaluation period used in this study (1998 - 2015),

this database contains 9.8 million pCO_2 observations within the coastal domain. All data from SOCATv6 are converted from

fugacity of CO_2 in water to pCO_2 using the formulation of Takahashi et al. (2012). We finally compare the pCO_2 simulated by

the MOM6-COBALT model to the 0.25° continuous monthly pCO_2 fields generated from the SOCAT observations by the

135   two-step neuronal network (SOM-FFN) in coastal regions (Laruelle et al., 2017). The SOM-FFN data product of Laruelle et

al. (2017) is thus not "raw" and implies a significant amount of statistical modelling. It is also derived from an earlier version

of SOCAT (SOCATv4, Laruelle et al., 2017) than the "raw" one. In what follows, the pCO_2 products generated by the model,

the statistical interpolation of observations, and the un-interpolated observations will be referred to as MOM6-COBALT,

coastal-SOM-FFN and Socatv6, respectively. All observational and simulated fields are converted from their original spatio-

140   temporal resolution to monthly 0.25° gridded climatologies for the 1998 - 2015 period to match the one used by the coastal-

SOM-FFN. Cells that are covered by more than 95 % of sea-ice are removed from the comparison since we assume no transfer

of our master variable (pCO_2) through sea ice. In our analysis, we apply the broad definition of the coastal zone by Laruelle et

al. (2017), using a global mask that excludes estuaries and inland water bodies while its outer limit is set 300 km away from

the shoreline. This definition leads to a total surface area of 77 million km² which is split into 45 coastal regions using the

145   MARgins and CATchment Segmentation (MARCATS, Laruelle et al., 2013). These 45 regions are grouped into 7 broad

classes with similar hydrological and climatic settings (Liu et al., 2010): (1) Eastern and (2) Western Boundary Currents (EBC

and WBC respectively), (3) tropical margins, (4) subpolar and (5) polar margins, (6) marginal seas and (7) Indian margins.

The model evaluation of all gridded environmental variables including pCO_2 is performed for the annual mean and the seasonal

150   cycle both globally and within each of the 45 MARCATS regions. For the seasonal analysis, for each variable, a climatological

monthly anomaly is calculated as the difference between the variable x for a given month and its climatological annual mean.

The evaluation of the seasonal amplitude is then performed using the bias between observed and simulated root mean square

(RMS) of their monthly anomalies. A positive bias represents a larger simulated seasonal amplitude than derived from the

observations. The temporal shift between observed and simulated seasonal cycles is also assessed from the Pearson correlation

155   coefficient (no units) of the regression between monthly times series simulated by MOM6-COBALT and those extracted from

the observations. These comparisons not only serve to assess the overall model's performance in reproducing observations but

also help identifying potential discrepancies between observed and simulated environmental fields (e.g., SST, SSS) that are

used by the two-step neuronal network coastal-SOM-FFN to generate the continuous pCO_2 climatology.

160   Finally, from this global and regional spatio-temporal evaluation, we label the model skill ('high', 'medium' and 'low') for

each MARCATS and identify regions for which our results are the most robust for further in-depth analysis of the processes

driving the coastal pCO_2 dynamics. The model skill labelling is based on 3 criteria: First, we assess whether the simulated

annual mean pCO_2 is within 20 µatm of the one extracted from the coastal-SOM-FFN. This threshold of 20 µatm roughly

corresponds to the globally averaged pCO_2 gradient between the atmosphere and the coastal sea surface (Laruelle et al., 2018).

165 The second and third criteria evaluate the magnitude and phasing of the simulated pCO_2 seasonal cycle against the coastal-SOM-FFN, using an absolute bias in the seasonal magnitude < 20 µatm and a Pearson coefficient > 0.5 as threshold. Model skill is considered 'high' when the 3 criteria are fulfilled, 'medium' when criteria 2 and 3 are satisfied and 'low' when only one or zero criteria is met on the seasonality.

2.3 Processes controlling seasonal pCO_2 variability: a method tailored for coastal regions

170 pCO_2 in surface sea water can be computed from DIC and ALK following Eq. (1) (Sarmiento and Gruber, 2006; Wolf-Gladrow et al., 2007):

$$pCO_2 = \frac{K_2'}{K_0' K_1'} \cdot \frac{(2DIC - ALK)^2}{ALK - DIC} \tag{1}$$

175 where K_0' is the aqueous-phase solubility constant of CO_2 in water and K_1' and K_2' represent the apparent equilibrium dissociation constants of the carbonate system. Several physical and biogeochemical processes can thus affect pCO_2 via changes in DIC, ALK and/or via the $\frac{K_2'}{K_0' K_1'}$ term which depends on SST and SSS. To quantify the processes controlling the pCO_2 variability at the seasonal timescale of interest to this study, we adopt the method of Liao et al. (2020). The method starts from the traditional approach that links variations in sea surface ocean pCO_2 to changes in DIC, ALK, SST and SSS using the

180 following linear decomposition (Doney et al., 2009; Lovenduski et al., 2007; Takahashi et al., 1993; Turi et al., 2014):

$$\Delta pCO_2 \approx \frac{\partial pCO_2}{\partial DIC} \Delta DIC + \frac{\partial pCO_2}{\partial ALK} \Delta ALK + \frac{\partial pCO_2}{\partial SST} \Delta SST + \frac{\partial pCO_2}{\partial SSS} \Delta SSS \tag{2}$$

Where the "Δx" terms represent the seasonal anomaly of x (i.e. the departure from the annual mean) and $\frac{\partial pCO_2}{\partial DIC}$, $\frac{\partial pCO_2}{\partial ALK}$, $\frac{\partial pCO_2}{\partial SST}$

185 and $\frac{\partial pCO_2}{\partial SSS}$ are coefficients that describe the sensitivity of pCO_2 to changes in DIC, ALK, SST and SSS. The coefficients for DIC, SST and SSS are always positive as pCO_2 increases with increases in DIC, SST or SSS, while the coefficient for ALK is always negative as pCO_2 systematically decreases with increasing ALK. These coefficients are generally estimated using the approach of Sarmiento and Gruber (2006) (see Eq. S1-S4 in Appendix), which has been widely used in the open ocean (Liao et al., 2020; Sarmiento and Gruber, 2006; Takahashi et al., 1993). In this study, we refine the estimation of the coefficients so

190 they can be used for the wide range of DIC/ALK ratios that can be encountered in the coastal waters. This includes conditions when the DIC/ALK ratio is close to 1, such as in regions with significant freshwater discharge like those found near estuarine mouths or on polar shelves subject to sea-ice melting, when pH is around 7.5 (Egleston et al., 2010). In these case, the traditional approximation method breaks down (see Eq. (S1-S2) and Figure S1 in the Appendix). To circumvent this important limitation, we computed the coefficients of the pCO_2 dependency using a regression approach based on the CO2SYS program

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195 (Lewis and Wallace, 1998). At each point in space, pCO_2 was computed using the 1998 - 2015 average of DIC, ALK, SSS and

SST with CO2SYS (method 14 in CO2SYS Matlab program, Millero, 2010). The $\frac{\partial pCO_2}{\partial DIC}$ coefficient was then computed as the

slope of the linear regression between pCO_2 and DIC obtained by allowing DIC to vary around the local mean DIC value while

keeping other tracers (ALK, SST, SSS) constant. The DIC range used to compute the slope was set to the ± 2 standard deviation

of the 1998-2015 monthly values at that location with an upper bound at ± 60 µmol kg^{-1} (see Appendix for further details).

200 The same approach was repeated to compute the coefficients for the pCO_2 dependence on ALK, SST and SSS, respectively.

Our methodology leads to coefficients that are constant in time but space dependent. In Fig. S1, we compare the coastal pCO_2

reconstructed from the traditional decomposition (using the empirical coefficients reported by Sarmiento and Gruber, 2006)

with those computed here. For the global coastal ocean, we find a large bias (global mean rmse of fitting pCO_2 anomaly in Eq.

(2) = 14.6 µatm), which is especially pronounced at high latitudes. In contrast, the decomposition method based on our

205 methodology reduce drastically the biases (global mean rmse = 2.8 µatm) in coastal regions and allows a more robust

reconstruction of the pCO_2 variability.

Here we assume that the coefficients are constant in time, and the temporal change in pCO_2 ($\partial_t pCO_2$ in µatm month^{-1}) can

therefore be expressed as a simple function of the temporal changes in DIC ($\partial_t DIC$), ALK ($\partial_t ALK$), SST ($\partial_t SST$) and SSS

210 ($\partial_t SSS$):

$$\partial_t pCO_2 \approx \frac{\partial pCO_2}{\partial DIC}\partial_t DIC + \frac{\partial pCO_2}{\partial ALK}\partial_t ALK + \frac{\partial pCO_2}{\partial SST}\partial_t SST + \frac{\partial pCO_2}{\partial SSS}\partial_t SSS \tag{3}$$

Temporal changes in DIC, ALK, SST, and SSS ($\partial_t DIC$, $\partial_t ALK$, $\partial_t SST$ and $\partial_t SSS$) are controlled by surface heat flux, ocean

215 transport, freshwater fluxes, biological processes, and the air-sea CO_2 flux. Using the model results, we further expand the

decomposition to quantify the contribution of these physical and biological processes (see details of derivation in Liao et al,

2020) :

$$\underbrace{\partial_t pCO_2}_{pCO_2\ change} \approx$$

220 $$\underbrace{\left(\frac{\partial pCO_2}{\partial DIC}\partial_t DIC_h + \frac{\partial pCO_2}{\partial ALK}\partial_t ALK_h + \frac{\partial pCO_2}{\partial SSS}\partial_t SSS_h + \frac{\partial pCO_2}{\partial DIC}\partial_t DIC_v + \frac{\partial pCO_2}{\partial ALK}\partial_t ALK_v + \frac{\partial pCO_2}{\partial SSS}\partial_t SSS_v\right)}_{circ}$$

$$+ \underbrace{\left(\frac{\partial pCO_2}{\partial DIC}\partial_t DIC_{fw} + \frac{\partial pCO_2}{\partial ALK}\partial_t ALK_{fw} + \frac{\partial pCO_2}{\partial SSS}\partial_t SSS_{fw}\right.}_{fw}$$

$$+ \underbrace{\left(\frac{\partial pCO_2}{\partial DIC}\partial_t DIC_{bio} + \frac{\partial pCO_2}{\partial ALK}\partial_t ALK_{bio}\right)}_{bio}$$

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$$+ \underbrace{(\frac{\partial pCO_2}{\partial T} (\partial_t SST_h + \partial_t SST_v + \partial_t SST_q)}_{thermal}$$

$$+ \underbrace{(\frac{\partial pCO_2}{\partial DIC} \partial_t DIC_{CO_2\ flux})}_{CO_2\ flux} \tag{4}$$

225

where the temporal changes in pCO₂ (time tendency called *pCO₂ change*) is on the left-hand side (LHS), and the five terms that control this change in pCO₂ are on the right-hand side (RHS) of the equation. Subscripts *h* and *v* denote the contribution from horizontal (advection and diffusivity in the meridional and zonal directions) and vertical (vertical advection and diffusivity) transports on SST, SSS, DIC and ALK, *bio* denotes the DIC and ALK changes induced by biological processes

230 (photosynthesis, respiration, and calcium carbonate dissolution/precipitation, denitrification and nitrification), *q* denotes the effect of surface heat flux on SST, *fw* denotes the effect of fresh water fluxes (i.e., precipitation, evaporation, river runoff and sea-ice formation and melting) on SSS, DIC and ALK, and the term *CO₂ flux* denotes the DIC change induced by air-sea CO₂ exchange.

235 Here we examine changes in pCO₂ attributed to three oceanic processes that modify the concentration in dissolved species (i.e. DIC, ALK and SSS), namely their transport by oceanic circulation (*circ*, which include horizontal and vertical transport), the effect of dilution/concentration due to freshwater fluxes (*fw*) and the effect of biological activity (*bio*), and isolate the *thermal* influence tied to SST changes induced by both oceanic transport and air-sea exchange of heat. Finally, the air-sea CO₂ exchange (*CO₂ flux*) pushes the surface pCO₂ concertation towards its equilibrium with the atmosphere and systematically acts to offset

240 the pCO₂ changes associated with the sum of the internal oceanic processes (*circ*, *bio*, *fw* and *thermal*). In this study, we apply Eq. (4) using averages between the sea surface and the mixed layer depth (MLD), defined here as the depth where the water density is 0.01 kg m⁻³ denser than the water at the surface (minimum MLD is 5 meters). Positive contributions on the RHS would yield an increase in pCO₂ (positive pCO₂ response on the LHS). Positive values of the *CO₂ flux* correspond to an ocean CO₂ uptake. This method to decompose the pCO₂ seasonality into controlling processes in the coastal domain is illustrated in

245 three coastal regions: The East and West coast of North America and in the Norwegian Basin.

3 Results and discussion

3.1 Annual mean state and seasonal cycle model evaluation and identification of coastal regions

Figure 1a identifies the coastal regions where the performance of MOM6-COBALT is satisfactory for both the annual mean and the seasonal cycle of pCO₂. The analysis, performed at the MARCATS scale (see Fig. 1b for nomenclature), distinguishes

250 regions of low, medium and high model skill, the latter being areas for which our confidence in the identification of the dominant biophysical drivers of the coastal pCO₂ dynamics is highest. This figure will be analyzed in detail in Section 3.1.3, but before we do so we first perform a data-model evaluation according to the following: We first evaluate the model by

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comparing simulated fields of SSS, SST, sea surface nutrients to observations globally and regionally (Sect. 3.1.1, Figs. 2 and
3). Second, the ability of the model to capture the coastal pCO_2 annual mean and seasonality is assessed against the "raw"
255   Socatv6 data and the continuous monthly observational-based pCO_2 product (coastal-SOM-FFN, Laruelle et al., 2017),
respectively (Sect. 3.1.2, Figs. 3-6).

3.1.1 Model evaluation for coastal waters environmental variables

MOM6-COBALT captures fairly well the main spatial patterns of key environmental parameters (SST, SSS and sea surface
nutrients) in the coastal domain (Fig. 2). The global SST field simulated by the model reproduces the strong large-scale tropical
260   to polar SST gradients, with a global median bias of -0.2 °C (Fig. 2a-c), and biases at the scale of MARCATS regions ranging
from 0 °C in the North East Atlantic (M17) to 1.3 °C in the East coast of the U.S (M10, Fig. 3a and Table S1). With a global
median bias value of 0.2, the model also correctly reproduces the observed SSS patterns which are mainly regulated by
evaporation and freshwater inputs from precipitation, riverine runoff and ice melt, with lower SSS values in polar regions and
along the coasts in Southeast Asia and higher SSS values along the coasts of evaporation basins such as in the Arabian or the
265   Mediterranean Sea (Fig. 2d-f). The SSS analysis at the MARCATS scale reveals absolute SSS biases generally less than or
close to 1 except for five MARCATS where absolute biases exceed 2. These MARCATS are mainly located in marginal seas
(the Baltic Sea, M18, the Black Sea, M21 and the Persian Gulf, M29), but also include one polar region (the Canadian
Archipelago, M13) and one tropical region (Tropical West Atlantic, M7, Fig. 3b and Table S1). Similar to SSS, largest model-
data discrepancies for nutrients are mostly found in marginal seas (Fig. 3c-e and Table S1). For instance, the largest PO_4 and
270   SiO_4 biases are encountered in the Black Sea (M21, absolute biases of 3 and 75 µmol kg^{-1}, respectively). The Peruvian
upwelling (M4), the Bay of Bengal (M31) and the N-E Pacific (M1) also present large biases in NO_3 and PO_4, respectively
(e.g., NO_3 bias of 8 µmol kg^{-1} for M4). The global median nutrients biases are however much smaller, reaching 0.3, -0.2 and -
0.4 µmol kg^{-1} for nitrate (NO_3, Fig. 2i), phosphate (PO_4, Fig. 2l) and silicate (SiO_4, Fig. 2o), respectively,

The model-data seasonal evaluation reveals that MOM6-COBALT reproduces the global SST and SSS amplitudes remarkably
275   well (median absolute bias of 0.1 °C and 0.0, respectively, Table S2). Some exceptions can nevertheless be diagnosed such as
in the marginal Black Sea (M21) where the bias in SST seasonal amplitude reaches -1.3 °C, and in three MARCATS (The Bay
of Bengal (M31), the Tropical West Atlantic (M7), and the Siberian Shelves (M43)) where the SSS seasonal biases are larger
than 0.4. The model-data comparison also reveals that the phasing of the SST and SSS seasonal cycles are in very good
agreement (Pearson correlation close to 1) for all 45 MARCATS but four, for which significant deviations in SSS are found:
280   two marginal seas (Hudson Bay, M12 and the Red Sea, M28) and along the Californian (M2) and Brazilian Currents (M6).
The nutrients analysis shows absolute global median biases in seasonal amplitude of 0.1, 0.0 and 0.7 µmol kg^{-1} for NO_3, PO_4
and SiO_4, respectively. Seven MARCATS present absolute biases larger than 1.5 µmol kg^{-1} mainly located in marginal seas
(Baltic Sea, M18 and the seas of Japan (M40) and Okhotsk (M41)), but also in polar (Siberian (M43) and Antarctic (M45)
shelves) and subpolar (N-E Pacific, M1) regions and in the Bay of Bengal (M31). The model-data comparison sometimes

285   shows significant phases shift in their seasonal signal (Pearson coefficient < 0.5), such as for MARCATS located in Indian
       and Tropical margins, marginal seas and EBCs.

3.1.2 Model evaluation for coastal pCO_2

The spatial distribution of the annual mean pCO_2 simulated by MOM6-COBALT is in good agreement with the observational
pCO_2 values extracted from the "raw" Socatv6 database with generally low pCO_2 values (blue colors) in temperate and high
290   latitudes and high pCO_2 values (yellow and red colors) in tropical and sub-tropical regions (contrast Fig. 4a with Fig. 4b). The
       model-data pCO_2 evaluation at the regional scale shows that 33 of the 45 MARCATS present absolute biases lower than 20
       µatm (Table S1). The regions where the bias exceeds this threshold include two EBC's (M2 and M4), two marginal seas (M40
       and M41), and one Polar (M45), subpolar (M42) and Tropical East Atlantic (M23) shelf. Note that in some MARCATS regions,
       in particular in marginal seas and Indian seas, there are no Socatv6 observations to perform the comparison (e.g. the Bay of
295   Bengal, M31, see Fig. 4b and Table S1). Hence, we also evaluate the performance of MOM6-COBALT against the continuous
       coastal-SOM-FFN pCO_2 product which uses a neural network interpolation method to fill data gaps and resolve the spatio-
       temporal coastal pCO_2 variability globally.

Our results show that MOM6-COBALT reproduces the main spatial features of the annual mean pCO_2 field captured by the
coastal-SOM-FFN product, as revealed by the relatively low globally averaged bias of 2.5 µatm (Figs. 4a and 4c). In both the
300   model and the SOM-FFN product, low coastal pCO_2 values are consistently found in temperate and high latitude regions in
       both hemispheres, while high pCO_2 values are largely limited to (sub)tropical regions. Largest discrepancies (Fig. 4d) are
       found at high latitudes (poleward of 60° N and 60° S, negative bias), along the Eastern Boundary Peruvian and Namibian
       upwelling systems (high positive bias) and more locally close to the mouth of some large rivers (e.g., the plume of the Amazon
       or the Rio de la Plata, high negative bias). We note however that these regions are poorly sampled in the Socatv6 dataset (Fig.
305   4b) and are thus likely weakly constrained in the coastal-SOM-FFN product (Fig. 4c).

At the regional scale, differences in annual mean pCO_2 between MOM6-COBALT and coastal-SOM-FFN are lower than 20
µatm in 35 MARCATS (Table S1, Fig. 3f), which partly is a reflection of the low annual mean biases observed in the
environmental driver variables in these regions (see Sect. 3.1.1). In EBC, WBC, and subpolar coastal regions, the model tends
to overestimate the regional mean pCO_2 compared to coastal-SOM-FFN (positive bias), except along the East coast of U.S
310   (M10), in the China and Kuroshio seas (M39) and in the North East Atlantic (M17, Table S1). In polar regions, the model
       generally underestimates the mean pCO_2 compared to coastal-SOM-FFN, except around the South of Greenland (M15). In
       Indian, marginal, and tropical coastal regions, no general trend can be identified regarding the sign of the bias, which can be
       positive or negative.

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315 Quantitatively, the 10 MARCATS with absolute biases > 20 µatm are mainly located in regions for which very limited or no observational data have been compiled in the Socatv6 database (Table S1) and/or for which large discrepancies can already be identified at the level of the master environmental variables (Sect. 3.1.1). These regions belong mainly to EBCs (3 out of the 6 EBC MARCATS), marginal seas (3 out of the 9 marginal seas MARCATS), the remaining four being either polar (M13 and M14), subpolar (M42) or Indian margins (M31). The largest biases are found in the Peruvian upwelling Current (M4), the South West of Africa (M24), the Californian upwelling Current (M2) and the Canadian Archipelago (M13) with biases of 106

320 µatm, 79 µatm, 35 µatm and -53 µatm, respectively.

Our analysis reveals that the seasonal amplitudes simulated by MOM6-COBALT are systematically larger than the ones estimated by the coastal-SOM-FFN product (Fig. 5a-b, red colors in Fig. 5c and positive biases in Table S2) for all coastal regions belonging to EBC, WBC, Indian and tropical margins. For the majority of polar and subpolar margins and for some marginal seas, the model simulates lower seasonal pCO_2 amplitudes (blue colors in Fig. 5c and negative biases in Table S2).

325 Note that the seasonal evaluation is only performed against the coastal-SOM-FFN product because only few 0.25° coastal cells (approximately 45) in the Socatv6 database contain complete continuous pCO_2 time series. Quantitatively, absolute biases between the modelled and coastal-SOM-FFN amplitudes do not exceed 20 µatm except for marginal seas where larger discrepancies are calculated (6 of the 9 marginal MARCATS, Table S2). The monthly mean pCO_2 seasonal cycle simulated by MOM6-COBALT is also well in phase (Pearson correlation coefficients > 0.5) with the one extracted from coastal-SOM-

330 FFN in 34 out of the 45 MARCATS (red colors in Fig. 5d and Table S2). The agreement is especially good in the best monitored MARCATS regions (MARCATS where > 50 % of the area is covered by Socatv6 observations, Table S1). For instance, in regions with good data coverage such as along the East coast of the U.S (M10, Fig. 6a), the Norwegian Basin (M16, Fig. 6b), the Californian Current (M2, Fig. 6c), the Leeuwin Current (M33), or the Brazilian Current (M6), the Pearson correlation coefficient is higher than 0.9 (Table S2). In contrast, the seasonal pCO_2 cycle simulated by MOM6-COBALT substantially

335 diverges from that of the coastal-SOM-FFN in four poorly monitored marginal seas (M12, M21, M28, M29) and in a few of the EBCs, Indian margins, subpolar margins (e.g., New Zealand, Fig. 6d) and tropical margins (Pearson correlation coefficient < 0.5, Table S2 and blue colors in Fig. 5d).

3.1.3 Identifying coastal regions of 'high' model skill

Overall, the pCO_2 spatio-temporal analysis model-data evaluation shows that out of 45 MARCATS, 29 have an absolute bias

340 for their annual mean < 20 µatm when MOM6-COBALT-coastal-SOM-FFN, MOM6-COBALT-Socatv6 and coastal-SOM-FFN-Socatv6 are compared (Table S1). Together, these 29 MARCTAS represent 65 % of the global coastal ocean surface area. For the 11 MARCATS that are best covered by observations (MARCATS where > 50 % of the surface area is covered by Socatv6 observations, Table S1), absolute biases for the annual mean are always < 20 µatm for the three product intercomparison, except in the Californian Current (M2), in the Baltic Sea (M18) and along the N-E Pacific (M1). The seasonal

345   MOM6-COBALT against coastal-SOM-FFN evaluation also reveal that 39 of the 45 MARCATS have pCO$_2$ seasonal
amplitude biases < 20 µatm and 34 MARCATS have a Pearson correlation coefficient > 0.5 (Table S2).

Based on this evaluation, we attribute for each MARCATS a level of confidence on the model skill ('high', 'medium' and
'low', Table 1 and Fig. 1a). Out of the 45 MARCATS, 25 are labeled as 'high' skill, that is to say, they fulfil the following
350   criteria regarding the annual mean and the seasonality (Table 1 and dotted MARCATS regions in Fig. 1a): a bias < 20 µatm
in the annual mean pCO$_2$ between MOM6-COBALT and coastal-SOM-FFN, a bias < 20 µatm in the magnitude of the seasonal
pCO$_2$ cycle and a seasonal phase characterized by a Pearson correlation coefficient > 0.5. Note that these MARCATS but M43,
M45, M1, M23 and M26 also present an annual mean pCO$_2$ bias < 20 µatm in the MOM6-COBALT-Socatv6 and coastal-
SOM-FFN-Socatv6 comparisons (Table S1). In addition, 7 'high skill' MARCATS also show a data density > 50 % (13
355   MARCATS if we lower the data coverage to > 30 %, Fig. 1a). These 7 MARCATS are located in contrasted coastal
environments, i.e. 3 EBCs (Iberian (M19) and Moroccan (M22) upwellings and the Leeuwin Current, M33), 1 WBC (East
coast of the U.S, M10), 1 Polar (Norwegian Basin, M16), 1 subpolar (NE Atlantic, M17) and 1 marginal sea (Gulf of Mexico,
M9). These 7 'high' skill MARCATS could also result from the very good correspondence on the data-model annual mean
and seasonal patterns in environmental fields (Table S1 and Table S2 except M22, M33 and M9 for the nutrient phasing) and
360   are therefore excellent potential candidates for an analysis of the processes controlling the coastal pCO$_2$ dynamics. 6 additional
MARCATS regions fulfil the criteria related to the seasonal pCO$_2$ evaluation while they fail to fulfil the annual mean pCO$_2$
bias threshold of 20 µatm. These 'medium' skill regions (Table 1 and dashed regions in Fig. 1a) include 2 EBCs (Californian
Current, M2 and SW Africa, M24), 1 marginal sea (Sea of Okhotsk, M41), 2 polar (Canadian Archipelago M13 and N
Greenland, M14) and 1 subpolar (NW Pacific, M42) shelves. The majority of marginal seas are systematically associated with
365   large biases whether on the pCO$_2$ or on the main environmental variables. These regions fulfill only one or no criteria regarding
the pCO$_2$ seasonality, and they are hence labeled as 'low' skill (Table 1, Fig. 1a). Other 'low' skill regions include 1 EBC
(Peruvian upwelling Current, M4), 1 Indian (Bay of Bengal, M31), 2 tropical (Tropical E Pacific, M3 and SE Asia, M38), 2
subpolar (Sea of Labrador, M11 and New Zealand, M36) and 1 WBC (Brazilian Current, M6) margins.

3.1.4 Methodological limitations

370   While our results show a relatively good agreement between MOM6-COBALT and coastal-SOM-FFN regarding the spatial
and temporal pCO$_2$ distribution over the global coastal ocean, the comparison remains challenging for several reasons.

First, while the climatology of Laruelle et al. (2017, coastal-SOM-FFN) is currently the best available product for a model-
data comparison, it has its own limitations. For instance, in some regions, particularly coastal upwellings such as the Moroccan
375   (M22) and Peruvian (M4) upwellings, the pCO$_2$ fields generated by the coastal-SOM-FFN do not reproduce well the high and
variable pCO$_2$ values measured in-situ (see e.g., Friederich et al., 2008 and McGregor et al., 2007). Such poor performance of
the coastal-SOM-FFN algorithm in these types of systems were already identified by Laruelle et al. (2017). Indeed, upwelling

regions are still relatively poorly monitored and expand partly beyond the coastal domain used by Laruelle et al. (2017), leading

to locally skewed calibration of the SOM-FFN. Deficiencies in the observation-based product can thus partly explain the large

380   model-data bias (106 µatm, largest of all MARCATS) calculated in the Peruvian upwelling region. Moreover, although the

Surface Ocean CO_2 Atlas database (SOCAT) has expanded significantly over the past few years, some regions are still poorly

monitored. In the coastal regions where no observational data exist (e.g., in the Black Sea, the Sea of Okhotsk, the Bay of

Bengal, Fig. 4b) in the SOCAT database used here (SOCATv6, Bakker et al., 2016), it is difficult to evaluate the performance

of the SOM-FFN and, thus, of an OGCM in reproducing the pCO_2 field. In addition, for certain regions subjected to complex

385   dynamic biogeochemical settings (e.g., upwelling, seasonal cover of sea-ice, influenced by rivers, marginal seas), the pCO_2

field reconstructed by the SOM-FFN suffers from poor performance, which can partly be explained by the lack of observational

data. This lack of observations could partly explain why MOM6-COBALT-coastal-SOM-FFN pCO_2 biases exceed 20 µatm

in these regions. This study highlights the regions (Fig.1a, e.g., Indian ocean margins, Peruvian upwelling, marginal seas)

where new observational data are most urgently needed to improve our understanding of the CO_2 exchange between coastal

390   regions and the atmosphere at the regional and global scales. In addition, only one global continuous pCO_2 climatology derived

by the SOM-FFN method currently exists for the coastal ocean. It would therefore be beneficial for the community to develop

other observation-based climatologies relying on other interpolation techniques, as currently the case for the open ocean.

Second, the model-data comparison should also be analyzed in the light of the current limitations in the model itself. OGCMs

395   have been designed for global ocean applications and the coarse spatial resolution of these models, on the order of 0.5° in the

present study, cannot resolve accurately mesoscale and sub-mesoscale processes as well as tidal mixing in shelf regions even

with a model configuration including parameterizations for these processes. The coastal currents are also not always well

resolved because of the coarse resolution of the shelf bathymetry. These small-scale hydrodynamic features are known to affect

the spatio-temporal variability of pCO_2 and the air-sea CO_2 exchange (Bourgeois et al., 2016; Kelley et al., 1971; Lachkar et

400   al., 2007; Laruelle et al., 2010). Therefore, although MOM6-COBALT runs at 0.5°, discrepancies between coastal-SOM-FFN

and MOM6-COBALT in narrow EBCs such as the Peruvian Upwelling Current (M4) and along South west Africa (M33)

could also be explained by the limited spatial resolution of the model. Moreover, OGCMs such as MOM6-COBALT have a

relatively simple representation of the biogeochemistry which does not fully captures some of the important processes of the

carbon dynamics in coastal waters such as sea-ice temporal dynamics (Adcroft et al., 2019), neritic calcification (O'Mara and

405   Dunne, 2019), or terrestrial and marine organic matter decomposition and burial (Lacroix et al., 2021). Moreover, the largest

biases observed in marginal seas can partly be explained by large fluvial inputs and oceanic water flows through fine scale

topography (e.g. straits) that are poorly represented in global OGCMs.

Finally, the annual mean/seasonal pCO_2 biases between the coastal-SOM-FFN and MOM6-COBALT can also be traced back

410   to divergences in the environmental fields simulated by the model compared to observations (Table S1 and Table S2). For

instance, in most marginal seas, the model poorly resolves the annual mean and seasonal cycle of SSS and nutrients compared

to the observations. These discrepancies impact the simulated pCO_2 via the controls of the SSS on the CO_2 solubility and of nutrients on the biological pump and CO_2 uptake. In the tropical W Atlantic (M7) which is under the influence of the Amazon River, the model simulates lower annual mean SSS (and therefore lower pCO_2) than the observations. In the tropical E Pacific

415   (M3) and in South-East Asia (M38), the poor agreement between simulated and observed seasonal pCO_2 cycle could be explained by significant biases in the nutrient seasonal cycles (low Pearson correlation coefficient). Interestingly however, some regions reveal significant biases in the major environmental fields but not in the pCO_2 (e.g., Tropical W Atlantic, M7) while in other regions, the reverse is observed (e.g., M20, M27 and M36). Also, for some regions biases in environmental fields do not affect the pCO_2 as expected. For instance, along the East coast of the U.S (M10), MOM6-COBALT simulates

420   larger SST compared to observations while the simulated pCO_2 is lower compared to coastal-SOM-FFN on an annual mean. This clearly shows that biases in environmental fields are not sufficient to explain fully the biases in pCO_2 diagnosed between MOM6-COBALT and coastal-SOM-FFN.

3.2 Processes governing the seasonal pCO_2 variability

Our second objective is to examine the drivers of the pCO_2 seasonality in three well sampled and contrasted coastal regions

425   where the model skill is satisfactory: The East coast of North America (M10), the Norwegian Basin (M16) and the Californian Current (M2). The East coast of North America is a sink of atmospheric CO_2 that has been extensively studied over the past decade (e.g., Fennel et al., 2019; Laruelle et al., 2015; Shadwick et al., 2010, 2011; Signorini et al., 2013). The pCO_2 spatio-temporal dynamics in this MARCATS is particularly well captured by MOM6-COBALT ('high' skill, Fig. 1a), despite an annual mean SST bias of 1.3 °C on the data-model comparison in this region (Table S1). Because the SST amplitude and

430   seasonal phasing are in agreement between the model and data (Table S2), the bias on the mean SST does not impact the seasonal pCO_2 cycle (Pearson correlation coefficient > 0.5 and bias < 20 µatm on the seasonal pCO_2 amplitude, Table 1). We also selected the Californian Current because it is a source of CO_2 to the atmosphere, and similarly to the East coast of the U.S, it ranks among one of the best monitored coastal regions in the world (e.g., Evans et al., 2011; Fennel et al., 2019; Hales et al., 2012; Turi et al., 2014). In this region, the model is classified as 'medium' skill (Table 1 and Fig. 1a). Indeed, the simulated

435   seasonal cycle of pCO_2 is in relatively good agreement with coastal-SOM-FFN (Figs. 5-6, and Table 1), despite biases in the annual mean pCO_2 compared to observations (Fig. 3f) and a phase shift in the seasonality of SSS and nutrients (Pearson correlation coefficient < 0.5). However, the Californian Current is also one of the few coastal regions where an analysis of the processes controlling the pCO_2 seasonality has already been performed using a regional biogeochemical model and sequential simulation removing processes one after the other (Turi et al., 2014), which can hence be compared to our analysis. Finally,

440   the choice of the Norwegian Basin is motivated by the good performance ('high' skill) of the model and the intense atmospheric CO_2 sink that occurs in this contrasted region.

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3.2.1 Seasonality along the East coast of North America

The seasonal evolution of pCO_2 averaged over the East coast of the U.S (M10) is represented in Fig. 7a. Ocean pCO_2 is minimum in winter (February/March ~ 331 µatm), it increases through spring and peaks in summer (August, ~ 400 µatm)

445 before decreasing again in the fall. Figure 7b reveals the complex interplay of the four ocean internal processes (thermal, biology, ocean circulation, and fresh water flux) on the seasonal pCO_2 variability which can either act in synergy or oppose each other.

The thermal effect (*thermal*, red line on Fig. 7b) increases pCO_2 from early spring to summer by decreasing the solubility of

450 CO_2. In contrast, the solubility of CO_2 increases in autumn and winter, inducing a decline in pCO_2. The largest changes in pCO_2 associated with the change in SST occur during spring (29 µatm month^{-1} in June) and fall (-26 µatm month^{-1} in November). This thermal effect was already identified by Signorini et al. (2013) in their observational study. These authors highlighted that lowest pCO_2 was generally reported in winter or at the beginning of spring and highest pCO_2 in summer or autumn, despite significant temporal and spatial heterogeneity between the different sub-regions of the East coast of the U.S

455 (Scotian shelf, the Gulf of Maine, the Georges Bank/Nantucket shoals, the Middle Atlantic Bight, and the South Atlantic Bight). The effect of biology above the mixed layer depth (*bio*, green line) reduces pCO_2 throughout the year revealing that primary production exceeds organic matter degradation in the surface layer all year long. The largest pCO_2 decrease associated with biology is observed in early spring (values of -68 µatm month^{-1} in April) which is well documented (e.g., Shadwick et al., 2010, 2011; Signorini et al., 2013). The transport of chemical species by ocean circulation (*circ*, blue line) increases pCO_2

460 and tends to oppose biology year-round except at the end of fall/beginning of winter. This pCO_2 increase induced by the circulation term is maximum in April (26 µatm month^{-1}). Throughout the year, the contribution of fresh water fluxes (*fw*, pink line) remains minor compared to the other terms (maximum absolute value of 9 µatm month^{-1} in January). For each month/season, the air-sea CO_2 exchange term (*CO_2 flux*, black line) counteracts change in pCO_2 associated with ocean internal processes taking place in surface seawater (sum of *bio*, *circ*, *thermal* and *fw*). The *CO_2 flux* term increases pCO_2 at the sea-

465 surface (acting as an atmospheric CO_2 sink) throughout the year except during summer (between July and September) where it decreases sea surface pCO_2 and releases CO_2 towards the atmosphere (acting as an atmospheric CO_2 source). This simulated atmospheric CO_2 uptake all year long except for the summer season is also in agreement with previous literature (Fennel et al., 2019; Laruelle et al., 2015; Signorini et al., 2013). The study of Laruelle et al. (2015) has nevertheless shown that in spring, the southern part of the Eastern North American coast is quasi neutral and that in fall, some regions such as the Gulf of Maine

470 or the Georges Bank acts as a CO_2 source. The temporal change of pCO_2 (*pCO_2 change*, cyan line) is the result of the non-perfect balance between the internal processes and the air-sea CO_2 flux.

We evaluate the rate of change tied to each process during the marked peak-to-peak pCO_2 increase observed between winter and summer (from 331 µatm in February to 400 µatm in August, Fig. 7a). A positive rate of change (in µatm month^{-1}) indicates

475 that the process contributes to an increase in pCO_2 between winter and summer (February-August). This process-based analysis reveals that the winter-to-summer pCO_2 increase in the East coast of the U.S (M10) mainly results from thermal (rate of change = +5 µatm month^{-1}) and ocean circulation (rate of change = +4 µatm month^{-1}) influences combined with a large reduction of the biological CO_2 uptake (rate change of +7 µatm month^{-1}, Fig. 7b). The importance of the thermal and circulation effects as well as the presence of a strong biological drawdown are in line with results from past studies (e.g., Laruelle et al. (2015),

480 Shadwick et al. (2010, 2011) and Signorini et al. (2013)). Our results which identifies the reduction of biological carbon uptake as a key control of pCO_2 seasonality agree with the studies of Shadwick et al. (2010, 2011), but slightly diverge compared to those of Signorini et al. (2013) or Laruelle et al. (2015), which found that the thermal effect was the dominant driver. This difference is largely explained by the different levels of details in the decomposition method. While most model studies, including ours, use seasonal change in SST, SSS, DIC and ALK, observational approaches cannot isolate the compounding

485 changes tied to biological activity from those of ocean transport.

3.2.2 Seasonality in the Norwegian basin and in the Californian Current

The pCO_2 seasonal cycle in the Norwegian Basin (M16) and the Californian Current (M2) simulated by MOM6-COBALT are represented in Fig. 7c and Fig. 7e, respectively. The Norwegian Basin shows a near-constant pCO_2 value (~ 330 µatm) throughout the year except in spring when it drops by 30 µatm (minimum pCO_2 value of 300 µatm in June). The phasing of

490 the seasonal pCO_2 cycle in the Californian Current is similar to that along the East coast of U.S, with a minimum pCO_2 value of 366 µatm in March followed by an increase that reaches a maximum pCO_2 value of 433 µatm in August and then decreases again at the beginning of the fall.

The decomposition of the seasonal cycle into different processes for both the Norwegian Basin and the Californian Current

495 (Fig. 7d and Fig. 7f) reveal patterns that are qualitatively similar to those already diagnosed for the East coast of the U.S (Fig. 7b). For both shelf regions, the biological and circulation effects respectively remain negative and positive throughout the year, while the thermal effect increases pCO_2 in spring and summer but decreases pCO_2 in fall and winter. The fresh water term is also minor compared to the other terms. Quantitatively, however, the amplitude of the different terms points to different first order control in the pCO_2 seasonality for each region. The amplitudes are calculated here using the marked peak-to-peak

500 change in pCO_2 which occurs between February and June in the Norwegian basin and between March and August in the Californian Current.

In the Norwegian basin, the strong winter to summer pCO_2 decreases (43 µatm, Fig. 7c) is mainly associated with the large and rapid CO_2 uptake associated with the spring phytoplankton bloom (biological rate of change = -45 µatm month^{-1} in average

505 between February and June and with a maximum pCO_2 uptake of -175 µatm month^{-1} in June, Fig. 7d). This biological drawdown is only partly compensated by the supply of high pCO_2 water masses by the ocean circulation (rate of change = +24 µatm month^{-1}). This dynamics is consistent with the fact that the Norwegian Basin is one of the most productive region of the

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world characterized by a well-documented, intense spring bloom (e.g., Findlay et al., 2008). In addition, the effect of thermal changes only plays a comparatively minor role here (rate of change = +7 µatm month^{-1}).

510

In contrast to the East coast of the U.S and the Norwegian Basin, the analysis performed in the Californian Current reveals that circulation is the main driver of the winter-to-summer pCO_2 increases (68 µatm, Fig 7e). The upwelling of high-pCO_2 waters increases surface pCO_2 year-round. Its influence is however weaker in winter than in summer, thereby explaining the pCO_2 increase observed between February and August (rate of change = +12 µatm month^{-1}, Fig. 7f). This large contribution
515   from circulation is consistent with the simulations of Turi et al. (2014), which identified the ocean transport associated with upwelling in the Californian Current as the dominant process, and the higher intensity of the summer upwelling and its impact on pCO_2 was also reported in prior work (e.g., Evans et al., 2015; Fiechter et al., 2014; Turi et al., 2014). In this region, biology also opposes the effect of ocean circulation, with upwelled deep water bringing nutrients to the surface and stimulating phytoplankton productivity (e.g., Evans et al., 2015; Fiechter et al., 2014; Turi et al., 2014). However, it plays a minor role in
520   the pCO_2 increase (rate of change ~ 0 µatm month^{-1}) as well as for the thermal effect (rate of change = +4 µatm month^{-1}).

4 Conclusions

In this study, an OGCM (MOM6-COBALT) which is primarily designed for the open ocean was used to examined sea surface pCO_2 seasonality in the coastal domain. We first evaluated the ability of the model to reproduce the spatial and temporal dynamics of key environmental variables, such as SST, SSS and sea surface nutrients against in-situ observations. The spatio-
525   temporal variability of coastal pCO_2 was also evaluated using direct coastal pCO_2 observations from the SOCAT database (Socatv6, Bakker et al., 2016), and a global observational continuous monthly pCO_2 climatology available at high spatial resolution (coastal-SOM-FFN, Laruelle et al., 2017).

Our model-data comparison showed a relatively good agreement on the environmental variables spatio-temporal distribution
530   except for some coastal regions mainly located in marginal seas. Our results also revealed a relatively good agreement between pCO_2 from MOM6-COBALT, coastal-SOM-FFN and Socatv6, both in time and space, and most of the discrepancies between the three products are found in regions with poor data coverage, such as in the Bay of Bengal, The Sea of Okhotsk or in the Hudson Bay (Fig. 1a). This study thus provides an objective framework to identify regions where new observational data collections are currently most needed to improve our global understanding of the CO_2 exchange between coastal regions and
535   the atmosphere. From the model-data evaluation, we identified regions where the MOM6-COBALT model shows highest skill in reproducing the spatial and seasonal pCO_2 variability, and where the different processes governing the pCO_2 dynamics can be examined with reasonable confidence ('high' and 'medium' skill regions in Table 1 and Fig. 1a).

We also adapted a novel method to quantify the contributions of the different physical and biological processes governing the

540 sea surface pCO_2 seasonality in the coastal domain. This method goes one step further than past coastal studies (e.g., Signorini et al., 2013; Turi et al., 2014) where the processes attribution was only based on the seasonal changes in DIC, ALK, SST and SSS or/and combined with a series of sequential simulations isolating one term after the other. In particular, our simulations are non-sequential and allow accounting for the co-variations between the different variables impacted by each process and how their simultaneous evolution modulates in quantitative terms the pCO_2 dynamics. Our approach, which is illustrated in

545 three coastal regions (the East coast of the U.S, the California Current and the Norwegian Basin), allows to decipher the complex interplay between ocean transport of chemical species (DIC, ALK and SSS), biological drawdown, fresh water fluxes (dilution/concentration effects) and thermal changes (air-sea fluxes and transport of temperature) on the pCO_2 dynamics. Depending on the season and region, these terms can reinforce or oppose each other and act to strengthen or dampen the amplitude of pCO_2 seasonal variations that control the air-sea CO_2 exchange. Along the East Coast of the U.S and in the

550 Californian Current, pCO_2 increases from winter-to-summer. In the former region, this increase is controlled by a subtle balance between biological drawdown, thermal changes and ocean circulation, while in the Californian Current, the circulation due to the upwelling (supplying pCO_2-rich waters to the surface) drives the increase in pCO_2. In contrast, in the Norwegian Basin, biological drawdown dominates the marked spring pCO_2 decrease observed in the region. These differences in the quantitative controls of pCO_2 dynamics from one region to another support our proposed analysis at the broad scale of the 45

555 MARCATS regions that together compose the global coastal ocean.

A handful of observational-based studies analyzed the seasonal variability of pCO_2 in the global coastal ocean (Cao et al., 2020; Chen and Hu, 2019; Laruelle et al., 2017). The mechanistic understanding of seasonal pCO_2 variations was, and remains limited by the amount of available observations. The modeling approach tailored for the coastal ocean presented in this

560 manuscript complements observational studies and help improve our quantitative understanding of the underlying physical and biological drivers of the coastal pCO_2 dynamics. The comparison of the model performance to a state-of-the-art coastal pCO_2 database and continuous pCO_2 data product also lends confidence in our model results for a large fraction of the global coastal domain. The coastal ocean is under tremendous anthropogenic pressure (e.g. climate, land-use change and agriculture, pollution, urbanization; e.g., Mackenzie et al., 2005; Regnier et al., 2013; Seitzinger et al., 2005). Understanding the interplay

565 between physics, biology and thermal processes and how they control coastal pCO_2 worldwide will be key to assess how their future changes impact air-sea CO_2 exchange in coastal environments.

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Data availability

575 The Surface Ocean CO_2 Atlas (SOCAT) is an international effort, endorsed by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS) and the Integrated Marine Biosphere Research (IMBeR) program, to deliver a uniformly quality-controlled surface ocean CO_2 database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT. Every previous version of the SOCAT database can also be accessed from the following page: https://www.socat.info/index.php/previous-

580 versions/. The coastal-SOM-FFN pCO_2 datasets description and dataset can be downloaded from Laruelle et al. (2017). The SST and SSS used for the evaluation the model were extracted from the NOAA OI SST V2 (Reynolds et al., 2007) and the EN4 SSS (Good et al., 2013), respectively. Nutrients data were extracted from the World Ocean Atlas 2018 (Garcia et al., 2019). The delineation and description of the MARCATS segmentation can be found in Laruelle et al. (2013).

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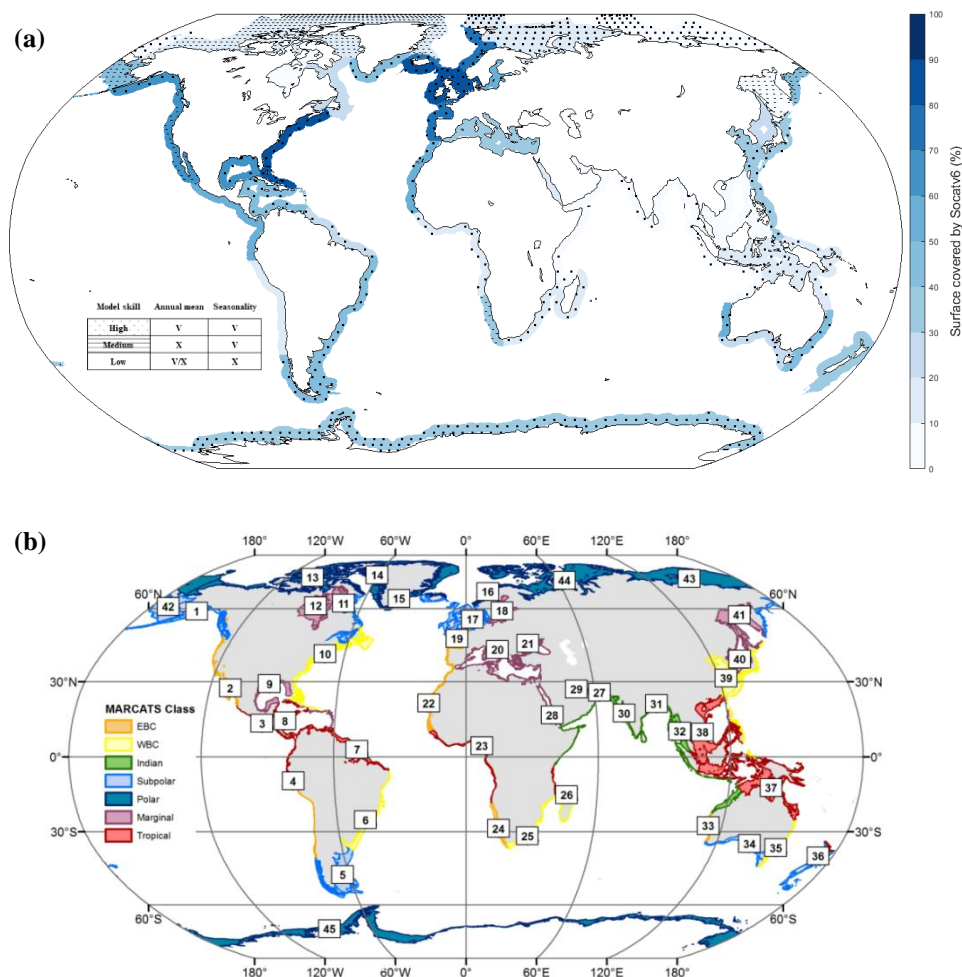
Figure 1: (a) Data coverage (color) and model skill (symbols) in coastal MARCATS (Margins and CATchment Segmentation) regions. The blue intensity indicates the fraction of the MARCATS' surface area covered by Socatv6 observations (from light to dark blue). Dots indicate where the model fulfils three evaluation criteria ('high' skill regions) on the spatio-temporal pCO_2 distribution (i.e., annual mean mismatch < 20 µatm between MOM6-COBALT and coastal-SOM-FFN, Pearson correlation coefficient > 0.5 and seasonal amplitude mismatch < 20 µatm). Dashes indicate where the model only fulfils two criteria (seasonal amplitude and phase, 'medium' skill). Other's regions ('low' skill with no symbol) do not fulfil the two criteria associated with seasonality. Details on model skill are in Table 1. (b) Discretization of the coastal seas into 45 MARCATS (Laruelle et al., 2013) grouped into seven classes: Eastern (MARCATS 2, 4, 19, 22, 24, and 33) and Western (MARCATS 6, 10, 25, 35, and 39) boundary currents (EBC and WBC, respectively), polar (MARCATS 13, 14, 15, 16, 43, 44, and 45) and subpolar margins (MARCATS 1, 5, 11, 17, 34, 36, and 42), tropical margins (MARCATS 3, 7, 8, 23, 26, 37, and 38), Indian margins (MARCATS 27, 30, 31, and 32), and marginal seas (MARCATS 9, 12, 18, 20, 21, 28, 29, 40, and 41).

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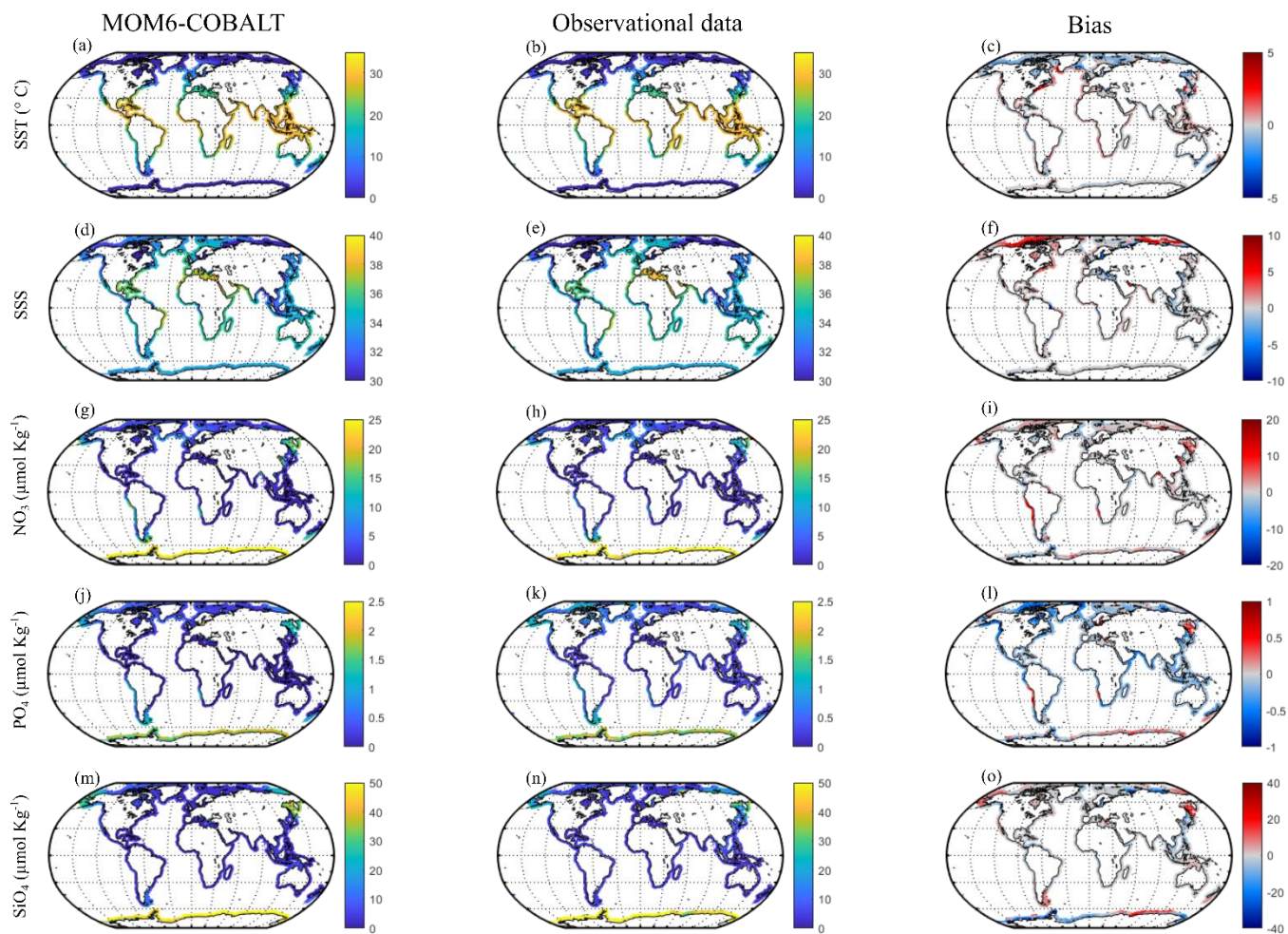
Figure 2: Observed (center) and modeled (left) spatial distributions of the annual mean state of SST (°C), SSS (no unit), nitrate (NO$_3$, μmol kg^{-1}), phosphate (PO$_4$, μmol kg^{-1}) and silicate (SiO$_4$, μmol kg^{-1}), and model annual mean bias (right). Observational SST and SSS fields are from the NOAA OI SST V2 (Reynolds et al., 2007) and the EN4 SSS (Good et al., 2013). Observational nutrients are from the World Ocean Atlas version 2018 (Garcia et al., 2019). The bias is the difference between MOM6-COBALT and observed values (red indicate regions where the simulated variables by MOM6-COBALT exceed observed values).

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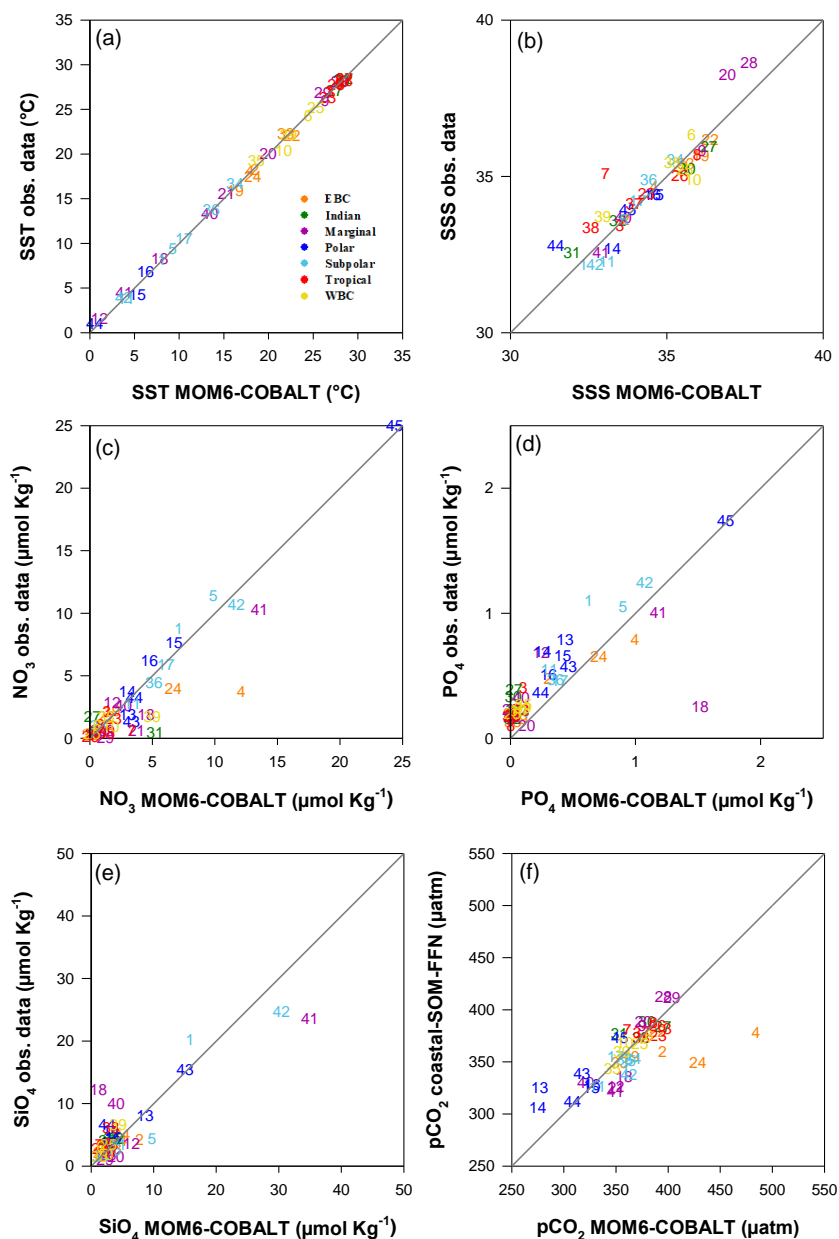
Figure 3: Comparison between observed and simulated annual mean fields in the 45 MARCATS regions: (a) SST (°C), (b) SSS (no unit), (c) NO₃ (μmol kg⁻¹), (d) PO₄ (μmol kg⁻¹), (e) SiO₄ (μmol kg⁻¹) and (f) pCO₂ (μatm). Observational datasets: SST and SSS are from the NOAA OI SST V2 (Reynolds et al., 2007) and the EN4 SSS (Good et al., 2013), nutrients are from the World Ocean Atlas 2018 (Garcia et al., 2019), pCO₂ is from the coastal-SOM-FFN product (Laruelle et al., 2017). Colors correspond to the seven major MARCATS classes (see Fig. 1b). In panels (d) and (e), the Black Sea (M21) is not represented and has a xy coordinated of (0.2; 3.5 μmol kg⁻¹) in panel (d) and (10.3; 83.1 μmol kg⁻¹) in panel (e). The Antarctic shelf (M45) is also not represented in panel (e) (55.0;49.1 μmol kg⁻¹).

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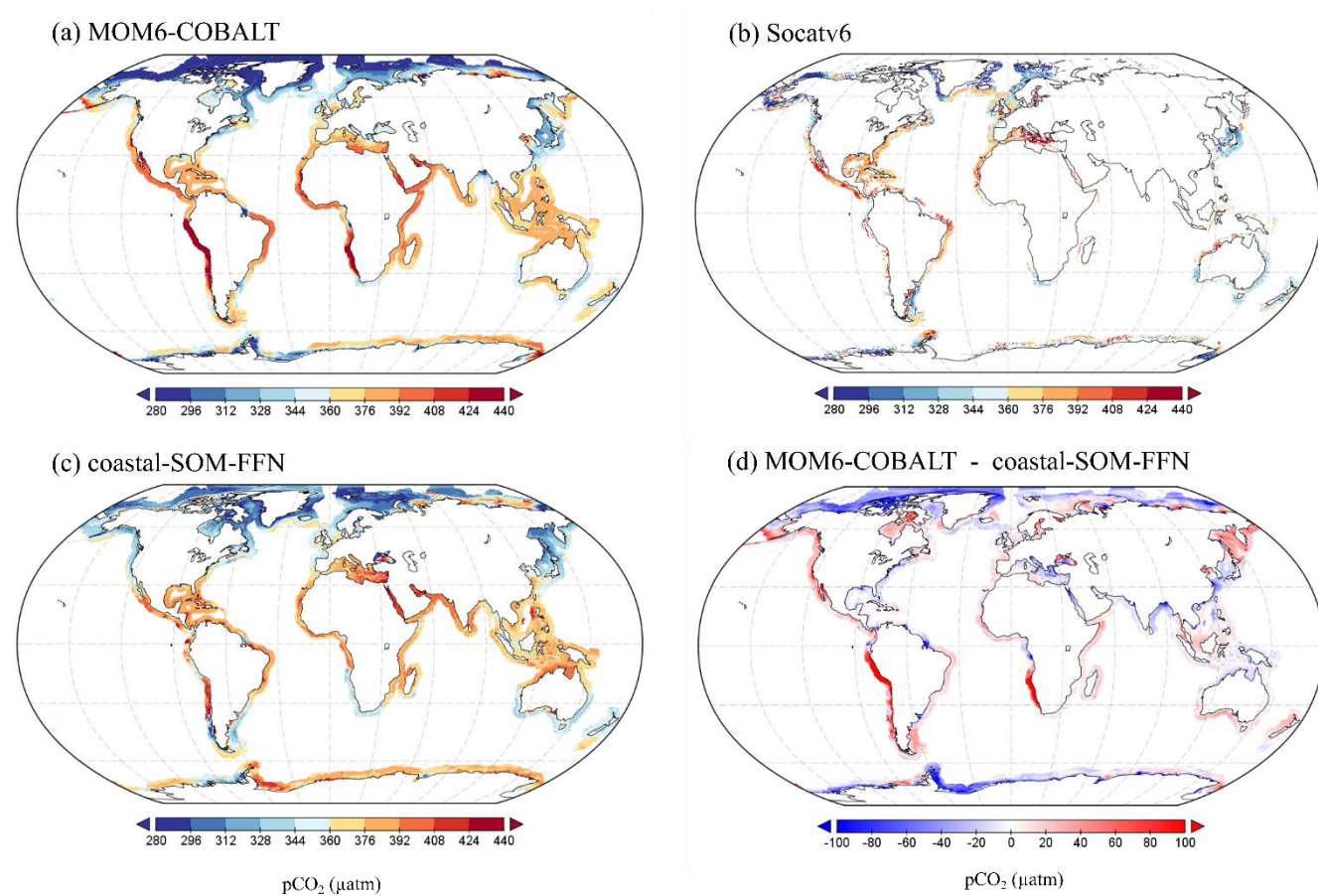
Figure 4: Spatial distributions of the annual mean pCO$_2$ (µatm) generated by (a) MOM6-COBALT, (b) extracted from the Socatv6 database and (c) from the coastal-SOM-FFN product (Laruelle et al., 2017). (d) Model bias as difference between panels (a) and (c) in µatm (red colors correspond to regions in which the pCO$_2$ simulated by MOM6-COBALT is higher than coastal-SOM-FFN).

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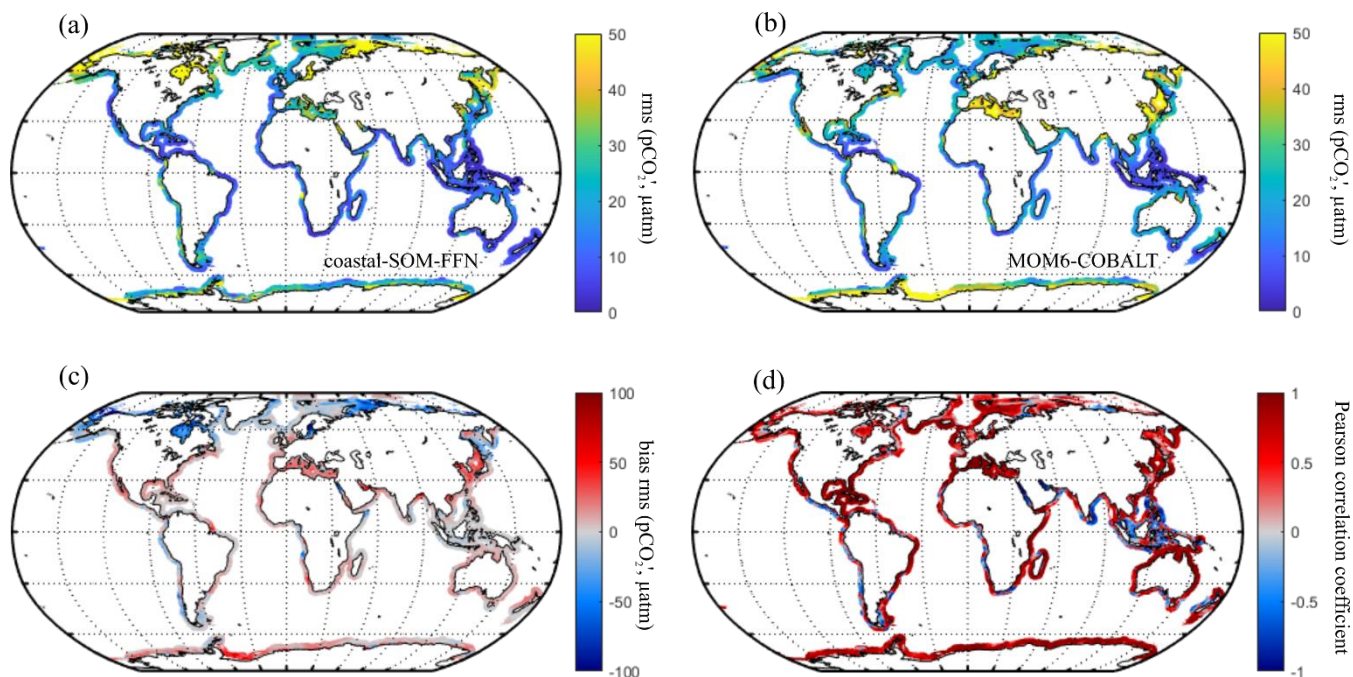
Figure 5: Seasonal variability in ocean pCO₂ (µatm). Seasonal amplitude (a) in the coastal-SOM-FFN product, (b) simulated by MOM6-COBALT model, (c) bias between model and coastal-SOM-FFN seasonal amplitude (red indicate simulated amplitude exceeds coastal-SOM-FFN). The seasonal amplitude is expressed as the root-mean-square of the monthly climatology pCO₂ anomalies ($RMS_{pCO_2'}$, µatm). (d) Pearson correlation coefficient of the regression between the seasonal pCO₂ cycles calculated by MOM6-COBALT and coastal-SOM-FFN. A value of 1 indicates that both signals are perfectly in phase with one another while a value of -1 represents a complete phase shift.

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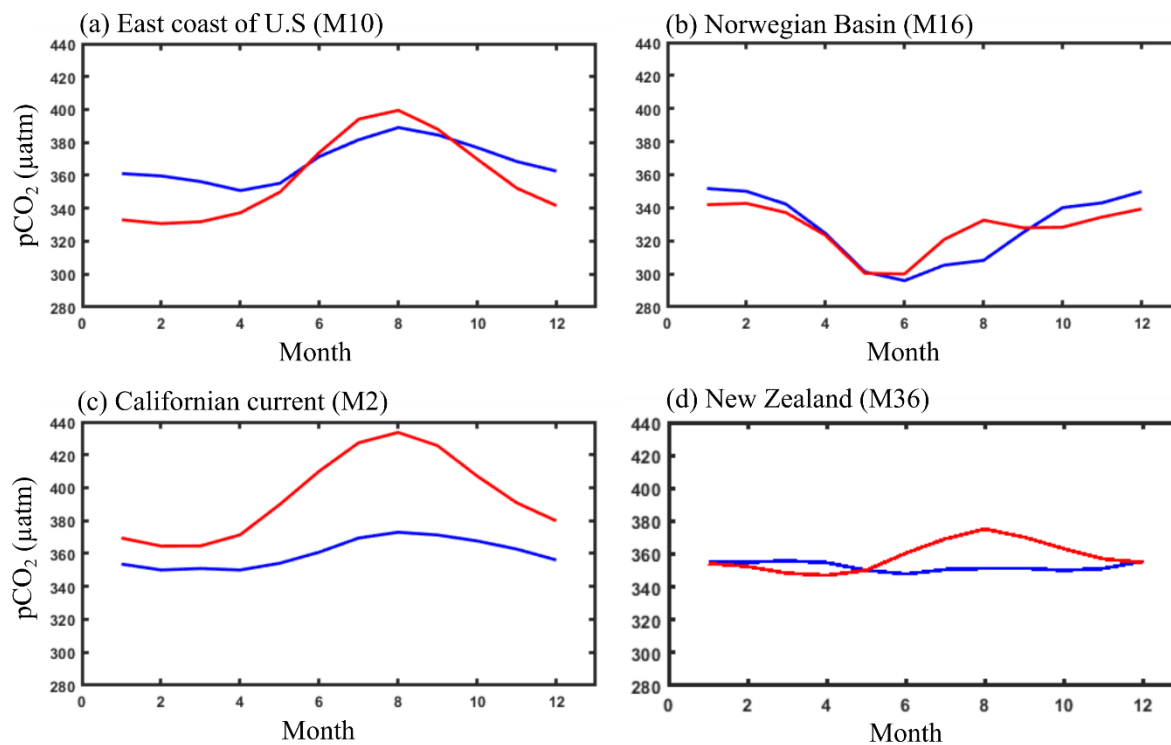
Figure 6: Seasonal pCO$_2$ cycle (µatm) derived from coastal-SOM-FFN (in blue) and simulated by MOM6-COBALT (in red) for (a) the East coast of the U.S (M10), (b) the Norwegian Basin (M16), (c) the West coast of North America (M2) and for (d) New Zealand (M36). Month 1 corresponds to January.

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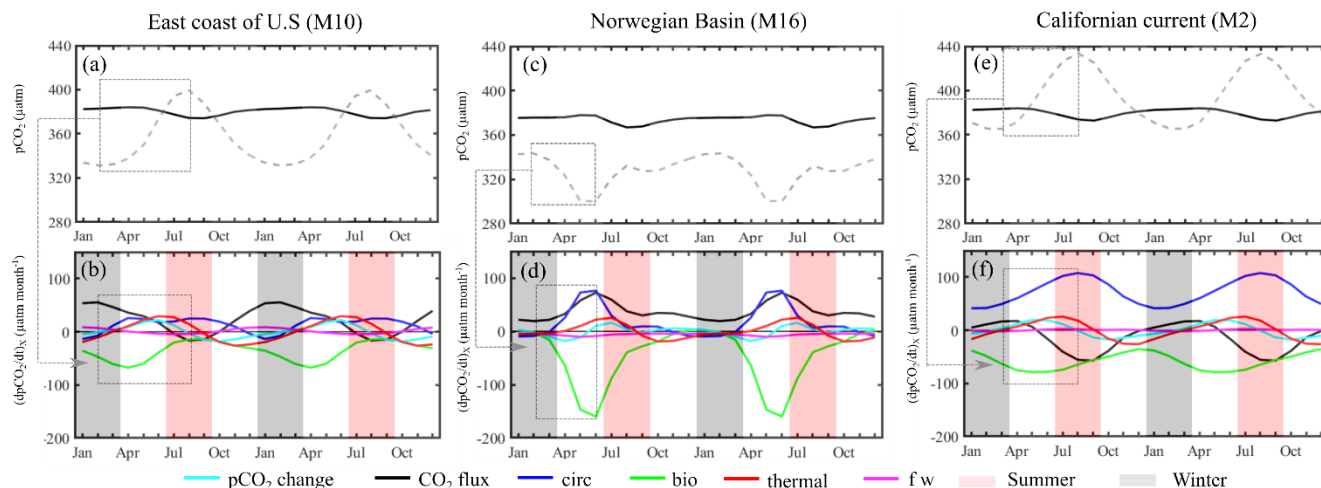
Figure 7: Processes controlling ocean pCO₂ seasonal cycle. Mean seasonal sea surface pCO_2 (dashed line) and atmospheric pCO_2 (black line) in µatm simulated by MOM6-COBALT and detrended over (a) the East coast of the US (M10) and (c) the Norwegian sea (M16) and (e) the Californian current (M2). Spatially averaged contributions (in µatm month^{-1}) from biological activity (*bio*, green), temperature changes (*thermal*, red), transport of chemical species (*circ*, blue), freshwater flux (*fw*, pink) and the CO_2 air-sea flux (*CO₂ flux*, black) controlling the pCO₂ temporal change (*pCO₂ change*, cyan) for the three regions (b, d and f). A positive value corresponds to an increase in sea surface pCO₂. Winter corresponds to the months of January, February and March, and Summer to the months of July, August and September.

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Table 1: Model skill level. For each MARCAT, the model skill ('high', 'medium' and 'low') is attributed from the pCO₂ spatio-temporal analysis. Regions where the model fulfils criteria on the annual mean and seasonality are labelled as 'high' skill regions (i.e., annual mean mismatch < 20 µatm between MOM6-COBALT and coastal-SOM-FFN, Pearson correlation coefficient > 0.5 and seasonal amplitude mismatch < 20 µatm, dots in Fig. 1a). High* skill region can present a bias > 20 µatm on the comparison with Socatv6 (see Table S1). 'Medium' skill regions represent MARCATS where the model only fulfils seasonal criteria (seasonal amplitude and phase, dashed in Fig. 1a). Other's regions ('low' skill) do not fulfil the two criteria associated to the seasonality (no symbol in Fig. 1a). Regions with 'high' model skill are considered as the most robust for an in-depth analysis of the processes driving the coastal pCO₂ dynamics and are highlighted in bold on the Table.

MARCATS number (Mx)	MARCATS name	MARCATS category	Annual mean pCO₂ (µatm)		Seasonal pCO₂			Model skill
					Amplitude (µatm)		Phasing (Pearson coefficient)	
			Coastal-SOM-FFN	Model bias	Coastal-SOM-FFN RMS	Model bias		
2	Californian Current	EBC	360.0	34.5	8.3	16.2	1.0	Medium
4	Peruvian upwelling Current	EBC	377.6	106.4	4.1	6.6	-0.4	Low
19	**Iberian upwelling**	**EBC**	**354.8**	**9.3**	**7.5**	**15.6**	**0.8**	**High**
22	**Moroccan upwelling**	**EBC**	**379.4**	**10.2**	**7.4**	**8.7**	**0.9**	**High**
24	SW Africa	EBC	349.1	79.3	7.2	4.2	0.9	Medium
33	**Leeuwin Current**	**EBC**	**349.4**	**4.2**	**5.6**	**12.7**	**0.9**	**High**
27	W Arabian Sea	Indian margins	383.5	11.6	8.7	3.6	0.3	Low
30	**E Arabian Sea**	**Indian margins**	**388.4**	**-8.3**	**4.8**	**6.2**	**0.7**	**High**
31	Bay of Bengal	Indian margins	377.3	-24.1	7.4	13.5	-0.2	Low
32	**Tropical E Indian**	**Indian margins**	**373.3**	**0.3**	**2.3**	**5.4**	**0.9**	**High**
9	**Gulf of Mexico**	**Marginal sea**	**384.3**	**-9.1**	**13.9**	**12.9**	**1.0**	**High**
12	Hudson Bay	Marginal sea	326.4	5.7	65.3	-46.4	0.4	Low
18	Baltic Sea	Marginal sea	336.2	21.4	79.4	-44.4	0.9	Low
20	Mediterranean Sea	Marginal sea	388.1	-11.9	25.1	20.6	1.0	Low
21	Black Sea	Marginal sea	325.0	25.2	141.9	-116.9	-0.5	Low
28	Red Sea	Marginal sea	412.2	-16.5	25.0	-0.4	-0.9	Low
29	Persian Gulf	Marginal sea	411.2	-7.6	31.3	30.7	-0.9	Low
40	Sea of Japan	Marginal sea	330.3	-9.3	21.1	28.0	0.9	Low
41	Sea of Okhotsk	Marginal sea	321.2	29.2	28.6	-6.5	0.7	Medium
13	Canadian Archipelago	Polar	325.4	-53.1	43.4	-18.0	0.9	Medium

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14	N Greenland	Polar	306.0	-24.3	21.7	-9.0	0.8	Medium
15	**S Greenland**	**Polar**	**325.2**	**1.3**	**24.5**	**-8.5**	**1.0**	**High**
16	**Norwegian Basin**	**Polar**	**328.1**	**-0.7**	**19.9**	**-6.1**	**0.9**	**High**
43	**Siberian Shelves**	**Polar**	**338.2**	**-19.7**	**57.4**	**-15.7**	**0.9**	**High***
44	**Barents and Kara seas**	**Polar**	**311.6**	**-3.3**	**24.9**	**-7.4**	**0.7**	**High**
45	**Antarctic Shelves**	**Polar**	**373.7**	**-17.6**	**22.6**	**13.3**	**1.0**	**High***
1	**N-E Pacific**	**Subpolar**	**342.5**	**16.8**	**15.8**	**-4.5**	**0.8**	**High***
5	**Southern America**	**Subpolar**	**351.1**	**14.0**	**12.1**	**-6.4**	**0.8**	**High**
11	Sea of Labrador	Subpolar	326.3	5.5	17.0	0.8	0.2	Low
17	**NE Atlantic**	**Subpolar**	**354.4**	**-4.5**	**14.9**	**-8.2**	**0.6**	**High**
34	**S Australia**	**Subpolar**	**352.7**	**13.5**	**3.7**	**12.8**	**0.9**	**High**
36	New Zealand	Subpolar	352.4	6.1	2.6	6.2	-0.5	Low
42	NW Pacific	Subpolar	337.7	25.2	36.5	-19.2	1.0	Medium
3	Tropical E Pacific	Tropical	382.2	17.2	6.9	3.1	0.3	Low
7	**Tropical W Atlantic**	**Tropical**	**380.3**	**-19.8**	**2.8**	**9.6**	**1.0**	**High**
8	**Caribbean Sea**	**Tropical**	**387.6**	**-1.7**	**6.6**	**2.2**	**1.0**	**High**
23	**Tropical E Atlantic**	**Tropical**	**374.6**	**15.9**	**2.9**	**1.5**	**0.6**	**High***
26	**Tropical W Indian**	**Tropical**	**384.8**	**4.8**	**7.1**	**5.6**	**0.9**	**High***
37	**N Australia**	**Tropical**	**378.5**	**-4.0**	**4.3**	**5.2**	**1.0**	**High**
38	SE Asia	Tropical	373.5	0.6	2.6	8.9	0.2	Low
6	**Brazilian Current**	**WBC**	**374.8**	**7.0**	**6.7**	**7.5**	**0.9**	**High**
10	**East coast of US**	**WBC**	**368.1**	**-9.6**	**12.0**	**12.4**	**0.9**	**High**
25	**Agulhas Current**	**WBC**	**367.1**	**5.7**	**7.1**	**8.1**	**1.0**	**High**
35	**E Australian Current**	**WBC**	**343.9**	**2.9**	**3.3**	**7.4**	**1.0**	**High**
39	**China Sea and Kuroshio**	**WBC**	**359.6**	**-4.1**	**10.3**	**13.2**	**0.9**	**High**

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